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Cross sections for electron-impact ionization of atoms and molecules and for electron-impact dissociation of molecules play an important role in determining the properties of electrical discharges, of the ionosphere and aurora, and of the plasmas that are widely used in microelectronics fabrication. The data base of these electron collision cross sections is very fragmentary or non-existent. This research has addressed these needs through the following accomplishments:

o Development, and application of a novel method for the measurement of accurate values of ionization cross sections of metal atoms.

o The discovery that the values of the ionization potential of C60 determined by the electron-impact and photoionization methods differ considerably indicating that low-lying metastable states are involved in the process. This may very well be the case for many other large molecules.

o Development of a time-of-flight, mass spectrometer of special design required for this effort.

o Development of a parallel adaptation of a computational procedure and its exploitation on large-scale parallel computers, consisting of hundreds of microprocessors, to generate electron-collision cross section data for gases relevant to plasma processing in semiconductor fabrication, e.g., PH3, AsH3, BCl3, CHF3, C2F6 and C4F8.

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Final Technical Report

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Laser Probing of Cross Sections for Ionization of Excited States and Molecular Dissociation by Electron Impact

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Abstract

Cross sections for electron-impact ionization of atoms and molecules and for electron-impact dissociation of molecules play an important role in determining the properties of electrical discharges, of the ionosphere and aurora, and of the plasmas that are widely used in microelectronics fabrication. The data base of these electron-collision cross sections is very fragmentary and non-existent. We have addressed these needs through the following accomplishments:

- Development and application of a novel method for the measurement of accurate values of ionization cross sections of metal atoms.

- The discovery that the values of the ionization potential of C_{60} determined by the electron-impact and photoionization methods differ considerably indicating that low-lying metastable states are involved in the process. This may very well be the case for many other large molecules.

- Development of a time-of-flight mass spectrometer of special design which was required for this effort.

- Development of a parallel adaptation of a computational procedure and its exploitation on large-scale parallel computers, consisting of hundreds of microprocessors, to generate electron-collision cross section data for gases relevant to plasma processing in semiconductor fabrication, e.g., PH_3, AsH_3, BCl_3, CHF_3, C_2F_6 and C_4F_8.

I. *Background and Objectives*

Cross sections for electron-impact ionization of atoms and molecules and for electron-impact dissociation of molecules play an important role in determining the properties of electrical discharges, of the ionosphere and aurora, and of the plasmas that are widely used in microelectronics fabrication. The data base of these electron-collision cross sections is very fragmentary and often non-existent. For example, with the exception of Ba, cross sections for electron-impact ionization of excited species have never been measured and data for electron-impact ionization of atoms in their ground states are not available for many species. Moreover, cross section data for electron-impact dissociation of gases into neutral fragments, a principal mechanism for generating the reactive species in plasmas, are not available for many gases of interest in microelectronics fabrication. These cross sections are among the most difficult to measure; unlike either positive or negative ions, quantitative detection of neutral dissociation products is very challenging.

The objectives of this effort were to address these needs through:

- Measurements of cross sections for electron-impact ionization of the ground and excited states of Li, Na, K, Ca, Sr, and Ba for impact energies from threshold to 1 KeV. Low-lying excited states of these atoms can be populated by lasers already available in our laboratory. Ba, Sr, Ca, and Li are of special relevance to the Air Force because they are released by the CRESS spacecraft designed to study the earth's ionosphere and magnetosphere.

- Measurements of ionization and attachment cross sections of excited states of SiH_4, I_2, NH_3, SO_2, and NO_2. These molecules have low-lying electronic states which are accessible with lasers in our laboratory.

- Calculations of the cross sections for electron-impact dissociation of gases into radicals for species of interest in etching plasmas used in microelectronics fabrication. Data for this principal process by which useful reactive species are generated in these plasmas are generally lacking. These cross sections are not only among the most difficult to measure but their calculation is computationally very intensive and has been beyond the reach of conventional computers for the polyatomic gases of interest. Our strategy has been to exploit large-scale distributed-memory parallel computers, consisting of hundreds of microprocessors, to generate electron collision data for feed gases such as $BC\ell_3$ and its fragments ($BC\ell_2$ and $BC\ell$), CF_3H, C_2F_6, and C_4F_8.

II. *Technical Summary*

(a) *Laser probing of cross sections for ionization of excited states and molecular dissociation by electron impact.*

We proposed to measure electron impact cross sections for the ground and excited states of many atoms and molecules which are found in Earth's atmosphere and for gases used in plasma processing of semiconductor materials. Specifically the following types of cross sections were proposed for measurement:

i) Ionization and dissociative ionization cross sections for the ground states.

ii) Similar cross sections for the excited states of some selected atoms and molecules.

iii) Cross sections for the production of negative ions.

iv) Cross sections for the production of neutral fragments from the dissociation of molecules.

For this purpose it was proposed to use a laser to: i) excite atoms or molecules to their excited states and then use routine methods of electron impact spectroscopy to measure cross sections, and ii) detect neutral fragments resulting from electron-impact dissociation of molecules by the method of laser-induced fluorescence (LIF).

In order to accomplish the proposed research an apparatus was assembled. It consisted of an electron gun of a special design, a mass spectrometer which was specifically developed for the present studies, an atomic and a molecular source for producing a beam of species under study, and a tunable ring dye laser (Coherent's Innova 100) which is considered top of the line for the present type of investigations. All these components were already available in our laboratory and, hence, any loss of time due to procurement was avoided.

The assembly and testing of apparatus took 6 months. A significant amount of time was spent aligning and tuning the laser to achieve the necessary stability in its operation. The first species studied by us was C_{60} molecule which was of great interest for space propulsion applications. The next six months were spent in studies connected with this molecule. A new property was discovered: It was found that ionization potential obtained by electron impact and by photo-absorption for the formation of doubly ionized species of this molecule differed considerably from each other. This finding was published in Rapid Communications in Mass Spectrometry.

Subsequently Na was studied. To make the measurements from the first excited state of Na, ionization cross sections from the ground state were needed. Accurate values of

these cross sections did not exist previously. Therefore, we developed a new method to accurately measure ionization cross sections for metal atoms. These cross sections were measured and published as a Rapid Communication in Physical Review A. Na was then excited to its first excited state by the tunable dye laser. To our surprise, we discovered that excited Na atoms associatively combine to give rise to Na_2^+ with great efficiency. This posed a major problem since we were interested in measuring ionization cross sections from the excited Na atoms. This associative ionization process depleted the population of excited Na atoms to the extent that a reasonable ionization signal could not be obtained. We spent a considerable amount of time in making this experiment work. However, we did not achieve results worth publishing.

In parallel we measured ionization, dissociative ionization and attachment cross sections for a number of species of interest to AFOSR. A list of papers published is attached here. We have data on cross sections for SF_6, F_2, H_2CO, S, and OCS. We are preparing these results for publication.

Some significant achievements include:

- We developed a new method for the measurement of accurate values of ionization cross sections of metal atoms.

- We discovered that the values of the ionization potential of C_{60} obtained by the electron-impact and photoionization methods differed considerably indicating that low-lying metastable states are involved in the ionization process. This may be true for many other molecules and should be systematically studied in the future.

- We developed a time-of-flight mass spectrometer of special design which was suitable for our studies.

(b) *Electron Collision Data for Plasma Modelling*

Plasma reactors are used in 30 to 40% of the processing steps in semiconductor fabrication. The cost of such semiconductor fabrication facilities is escalating, as is the research and development cost of introducing each new generation of plasma processing technology. It is now recognized that comprehensive three-dimensional, time-dependent simulations of these plasma reactors are essential to reducing the need for the costly and time-consuming experimental characterization currently required to develop a new generation of processing equipment. While such simulations have generally been beyond the reach of conventional supercomputers, large-scale parallel computers now have the potential to make them possible with industrially viable turnaround times.

While improved simulations of plasma reactors will depend on the availability of basic data for many processes in the plasma and at the surface, data for electron-molecule collisions, a principal mechanism for generating useful reactive species in these plasmas, are, however, especially important. As for many other processes in these plasmas, there are large gaps in the electron-collision data for gases of interest in microelectronics fabrication. Furthermore, cross sections for electron-impact dissociation of molecules into neutral fragments are among the most difficult to measure, many feed gases are hazardous, and transient fragments produced in situ may be experimentally inaccessible.

Computational approaches to obtaining such data are thus potentially of significant value. The collision of low-energy electrons with molecules is, however, a complex quantum mechanical problem. Calculating the probabilities of various possible outcomes of such a collision – that is, the scattering cross sections – is a correspondingly computationally intensive challenge. Hence, while several methods have been developed for numerical studies of such collisions, progress in their application to polyatomic gases of interest to plasma processing, e.g., species containing several carbon and halogen atoms, has been very limited. What is necessary to address this need in simulations of these plasmas for electron-collision cross section sets for multiple species is obviously a method of sufficient accuracy that is nonetheless computationally feasible for polyatomic feed gases.

In this effort we have exploited large-scale parallel computers, consisting of hundreds of microprocessors, to generate electron-collision cross section data for gases of interest in plasma simulations. In these studies we employ a parallel adaptation of a computational procedure based on a multichannel variational procedure which we specifically developed for studying low-energy electron-molecule collisions.[1] Like most variational schemes, the computational problem reduces to a set of linear equations – in matrix form, finding the unknown matrix $\mathbf{x}$ in the equation $\mathbf{A}\ \mathbf{x} = \mathbf{b}$. It is constructing, not solving, the linear system that is the computationally challenging part of our calculation.

Construction of this $\mathbf{A}$ matrix requires a quadrature approximation to an integral operator associated with the free-particle Green's function, which arises due to the boundary condition requirements of the collision. Since this quadrature is carried out over an infinite three-dimensional domain, tens of thousands of quadrature points may be required. At each quadrature point, we must evaluate all possible six-dimensional integrals of the form

$$\int\int d^3r_1\ d^3r_2 \frac{F_a(\mathbf{r}_1)F_b(\mathbf{r}_1)F_c(\mathbf{r}_2)\exp(i\mathbf{k}\cdot\mathbf{r}_2)}{|\mathbf{r}_1-\mathbf{r}_2|} \qquad (1)$$

Here, F_a, F_b, and F_c are Cartesian Gaussian functions, which are familiar to quantum chemists, and k is the quadrature variable. There are about $G^3/2$ unique ways to choose

the indices a, b, and c given a set of G Gaussians, so for G around 200 (typical in our work) we may need to evaluate as many as a few million such integrals at each of the quadrature points in $\mathbf{k}$. A large number of integrals ($\sim 10^9 - 10^{11}$) might hence be required in a cross section calculation.

Fortunately, the integrals in (1) can be evaluated analytically. This is no coincidence: Gaussians are used precisely because the resulting integrals are doable. Any single integral may therefore be obtained with little computational effort; what makes the problem numerically intensive is the vast number of integrals involved. However, it is not just evaluating all these integrals that is demanding. There are several intermediate steps in the process of building the elements of $\mathbf{A}$ and $\mathbf{b}$ from the integrals in (1), and the arithmetic associated with these steps often involves more operations than the actual computation of the integrals.

The outline of the numerical procedure is now obvious: first, evaluate a large number of integrals of the type shown in (1); next, combine those integrals in appropriate ways to construct matrices $\mathbf{A}$ and $\mathbf{b}$; finally, solve the resulting linear system. It is obvious that at least the first step in this procedure – evaluating a batch of integrals – is well suited to distributed-memory parallel machines such as the *Intel Paragon* and *Cray T3D*: We simply assign each processor a different subset of integrals to evaluate. Combining the integrals is more challenging, since the rules for building elements of $\mathbf{A}$ and $\mathbf{b}$ from the integrals are fairly complicated and the processors must communicate with each other in this phase (because each processor has only a fraction of the current batch of integrals in its own memory). An efficient way of carrying out this step is to use the complicated rules for combining integrals to build a single transformation matrix that, when multiplied with the current batch of integrals (arranged as a matrix) gives the necessary combination as a product matrix.[2] Each processor can build a block of this transformation matrix independently, so that the only communication among processors occurs during the matrix multiplication. A subsequent step in evaluating $\mathbf{A}$ – namely, the angular part of the quadrature over $\mathbf{k}$– can also be done as a matrix multiplication. In short, we can formulate both the evaluation and combination of the integrals in terms of procedures that are either perfectly parallel (involving no communication overhead) or highly efficient and relatively easy to program (multiplication of large, dense, distributed matrices). The remaining step, solving $\mathbf{A}\,\mathbf{x} = \mathbf{b}$ for $\mathbf{x}$, is straightforward.

The overall performance of our program on the *Intel Paragon* (512 processors) or *CRAY T3D* (256 processors) cannot be characterized by a single number. Although evaluating and subsequently combining the integrals are by far the dominant steps in the

calculation, the relative importance of these two steps is strongly dependent on factors such as the size of the molecule and the number of inelastic channels (processes) being considered. Depending on the nature of the calculation at hand and taking into account load balance, communication, I/O, and other overhead, we typically see throughput speeds in the range from 3 to 10 gigaflops. To put these numbers in perspective, our original sequential program, which is only partially vectorizable, averages about 30 megaflops on a Y-MP processor.

• This significant improvement in computational performance has greatly facilitated our efforts to obtain electron-collision cross sections for gases relevant to plasma processing in semiconductor fabrication, e.g., phosphine (PH_3), arsine (AsH_3), silane (SiH_4), tetrafluoromethane (CF_4), CHF_3, C_2F_6 and C_4F_8. We have also completed a project under the sponsorship of SEMATECH, Inc., to generate cross section sets for species relevant to boron trichloride ($BC\ell_3$) etching plasmas. These species included $BC\ell_3$ and its dissociation fragments ($BC\ell_2$ and $BC\ell$), as well as silicon tetrachloride ($SiC\ell_4$) and its fragments ($SiC\ell_3$, $SiC\ell_2$, and $SiC\ell$), which enter the plasma as products of the etch process. Since only limited experimental data are available for $SiC\ell_4$, and none at all to our knowledge, for the remaining molecules, these computations addressed a clear need.

• We have also completed calculations of the elastic and momentum transfer cross sections for collision of low-energy electrons with trimethylaluminum $(CH_3)_3$ $A\ell$. There is no electron collision data available for this species which is used in plasmas for deposition of aluminum nitride films and of aluminum metal on fibers for manufacture of fiber-reinforced composites, and for aluminum coating of the surface of ultra-fine particles. These results will also be used to put recent relative measured cross sections on an absolute scale.[3]

• In a joint effort with Professor Ehrhardt's group of Kaiserslautern University (Germany), we have carried out combined theoretical and experimental studies of the cross sections for electronic excitation of N_2 and CO by electron impact in the threshold region. Studies of such cross sections in the near-threshold region, which are often of greatest interest in simulations of weakly ionized plasmas, pose significant experimental and theoretical challenges. It is exactly in this region where available data is least reliable.

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Conferences and Conference Proceedings

1. *Formation of Positive and Negative Ions by Electron Impact on F_2*
M.V.V.S. Rao, I. Iga, and S.K. Srivastava
Book of Extended Abstracts of Contributed Papers in the XVIIIth International Conference on the Physics of Electronic and Atomic Collisions, eds. T. Anderson, B. Fastrup, F. Folkmann, and H. Knudsen (Aarhus University Press, Denmark, 1993), p. 338.

2. *Negative Ion Production from Electron Collisions with CS_2*
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3. *Electron Attachment to SF_6*
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4. *Cross Sections for the Formation of Negative Ions by Electron Impact on COS*
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5. *Electron Impact Ionization and Dissociative Ionization of C_2H_2*
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6. *Mass Spectrometric Study of Sulfur Vapor*
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- *Low Energy Electron Collisions with SF_6*, Invited Paper, 46th Gaseous Electronics Conference, Montreal, Quebec, October 1993.

- *Studies of Electron-Molecule Collisions on Highly Parallel Computers* , Invited Paper, 46th Gaseous Electronics Conference, Montreal, Quebec, October 1993.

- *Studies of Electron-Molecule Collisions on Parallel Computers*, Frontiers in Chemical Research Lecture, Texas A & M, December 1993.

- *Electron-Molecule Collisions for Modelling Materials-Processing Plasmas*, Invited Talk at Research Directors Conference, California Institute of Technology, February 1994.

- *Electron-Molecule Collisions for Modelling Materials-Processing Plasmas* , Invited Lecture at the Mardi Gras Conference: Towards Teraflop Computing, Louisiana State University, February 1994.

- *Electron-Molecule Collisions for Modelling Materials-processing Plasmas*, Invited Talk at the High-Performance Computing Symposium of the International Simulation Multiconference, La Jolla, April 1994.

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- *Electron-Molecule Collision Calculations for Modelling of BCl_3 Plasmas*, Invited Talk at the IEEE International Conference on Plasma Science, Santa Fe, June 1994.

- *Data for Modelling Materials-Processing Plasmas: The Impact of Parallel Computers*, Invited Talk at the Symposium on Applications of Advanced Innovative Computational Methods to Defense Science and Engineering, Institute for Defense Analyses, November 1994.

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- *Studies of Electron-Molecule Collisions on Highly Parallel Computers*, Seminar at the Geophysics Laboratory, Hanscom AFB, May 1995.

- *Studies of Electron-Molecule Collisions on Highly Parallel Computers*, Bucy Lecture, Texas Tech University, February 1995.

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- *Electron Impact Ionization and Dissociative Ionization of C_2H_2*, XIX International Conference on the Physics of Electronic and Atomic Collisions, British Columbia, August 1995.

- *Cross Section for Electron Collisions with H_2O*, Gaseous Electronics Conference, Berkeley, October 1995.

Personnel

Principal Investigator: Vincent McKoy, Professor of Chemistry
Co-Investigator: S.S. Srivastava, Research Scientist

K. Fujii, a Research Fellow, C. Winstead, a Senior Research Fellow, and C.-H. Lee, a graduate student were involved in this effort.